State-independent proof of Kochen-Specker theorem with 13 rays

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Quantum contextuality, as proved by Kochen and Specker, and also by Bell, should manifest itself in any state in any system with more than two distinguishable states and recently has been experimentally verified on various physical systems. However for the simplest system capable of exhibiting contextuality, a qutrit, the quantum contextuality is verified only state-dependently in experiment because too many (at least 31) observables are involved in all the known state-independent tests. Here we report an experimentally testable inequality involving only 13 observables that is satisfied by all non-contextual realistic models while being violated by all qutrit states. Thus our inequality will practically facilitate a state-independent test of the quantum contextuality for an indivisible quantum system. We provide also a record-breaking state-independent proof of the Kochen-Specker theorem with 13 directions determined by 26 points on the surface of a three by three magic cube.

It is believed, almost religiously, that every effect has its own cause and the same cause shall lead to the same effect. The predictions of quantum mechanics (QM) are however probabilistic and the effect that different outcomes appear in different runs of a measurement seem to have no definite cause, at least unexplainable using QM alone. Einstein, Podolsky, and Rosen [1] initiated a longlasting quest for a quantum reality by questioning the completeness of quantum mechanics. Hidden variable (HV) models are introduced in order to explain why a certain outcome appears in each run of a measurement, attempting to make QM complete. Years later Kochen, Specker [2], and Bell [3] discovered that quantum mechanics can be completed only by a hidden variable model that is *contextual*: the outcome of a measurement depends on which compatible observable might be measured alongside. Simply put, Kochen-Specker (KS) theorem states that non-contextual HV models cannot reproduce all the predictions of QM or quantum mechanics is contextual.

In any non-contextual HV model all observables have definite values determined only by some HVs λ that are distributed according to a given probability distribution ϱ_λ with normalization $\int d\lambda \varrho_\lambda = 1$. Two observables are compatible if they can be measured in a single experimental setup and a maximal set of mutually compatible observables defines a context. Non-contextuality is a typical classical property: the value of an observable revealed by a measurement is predetermined by HVs λ only regardless of which compatible observable might be measured alongside. Local realism is a form of non-contextuality enforced by the locality and thus Bell's inequalities [4] are a special form of KS inequalities [5–9], experimentally testable inequalities that are satisfied by all non-contextual HV models, some of which have been tested in recent measurements [10–18]. In general KS inequalities reveal the nonclassical nature of single systems demanding neither space-like separation nor entanglement, i.e., independent of state.
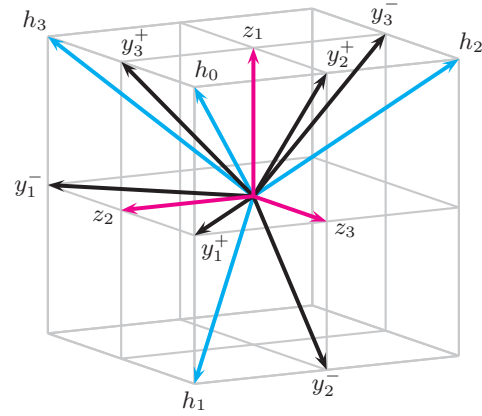

FIG. 1: (Color online) Illustration of 13 directions that are determined by 26 points on the surface of a 3×3 magic cube.

However for the simplest system capable of exhibiting the quantum contextuality, a qutrit, only a state-dependent verification has been made in a recent experiment [18]. This is because all the known state-independent KS inequalities for a qutrit [9] are based on the proofs of KS theorem and involve too many observables to be tested practically. For examples the original KS proof involves 117 directions [2] and Peres' [19] and Schuttle's [20] proofs involve 33 directions while the best KS proof known so far is due to Conway and Kochen [21] in which 31 directions are still involoved. Also there are many state-dependent KS proofs among which a 5-direction proof [7] has been used in the recent state-dependent experimental verification of quantum contextuality for qutrit. In this Letter we report a state-independent proof of KS theorem for qutrit with only 13 directions. Based on this proof we propose an experimental testable inequality that involves only 13 observables and two-observable correlations and is satisfied by all non-contextual HV models while being violate by all qutrit state. Thus our inequality will make a state-

independent test of quantum contextuality for an indivisible system practical.

How can we exclude non-contextual HV models for QM or prove the quantum contextuality? Obviously the answer depends on what kinds of quantum mechanical predictions we want the HV model to reproduce. For example if we only want the predictions on non-sequential measurements, i.e., correlations not included, to be reproduced, then a non-contextual HV model does exist according to Kochen and Specker [2]. Because of this toy model Kochen and Specker imposed a rather strong constraint on the HV models as a way out [2]: the algebraic structure of compatible observables must be preserved. Especially the value assigned to the product or the sum of two compatible observables must be equal to the product or the sum of the values assigned to these two compatible observables, which will be referred to as the product rule and the sum rule respectively. As we shall see later this constraint can be lifted if we consider sequential measurements.

As a result of the product rule the value assigned to the product of two orthogonal rays, normalized rank-1 projections, which are compatible, must be zero. As a result of the sum rule there is one and only one ray that is assigned to value 1 among all the rays in a complete orthonormal basis since the identity is always assigned to value 1. Thus in every non-contextual HV model preserving the partial algebraic structure of compatible observables there exists a *KS value assignment* to all rays in the corresponding Hilbert space satisfying:

1. The value $\{0, 1\}$ assigned to a ray is independent of which bases it finds itself in;

2. One and only one ray is assigned to value 1 among all the rays in a complete orthonormal basis.

The first condition reflects the non-contextuality and the second condition arises from the requirement that the algebraic structure of compatible observables be preserved. For a Hilbert space of a dimension greater than 2 there always exists a finite set of rays to which the KS value assignment is impossible. For qutrits, a state-independent proof originally involves 117 rays [2] and the number is reduced to 33 by Peres [19] and Schütte as reported by K. Svozil in 1994 and pointed out by Bub [20]. The best KS proof known so far is given by Conway and Kochen [21] with 31 rays. For 4-state systems the best state-independent proof is due to Cabello, Estebaranz, and García-Alcaine [22] with 18 rays, the smallest state-independent KS proof known so far.

To warm up let us present a state-independent proof of KS theorem for qutrit using only 13 rays. In a given basis $\{|0\rangle, |1\rangle, |2\rangle\}$ we shall represent a qutrit ray $\hat{r} = |r\rangle\langle r|/\langle r|r\rangle$ by a triple $r = (a, b, c)$ such that $|r\rangle = a|0\rangle +$
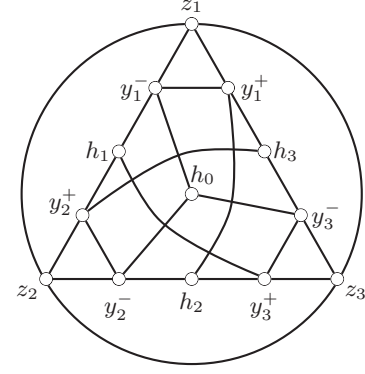

FIG. 2: The orthogonality relationships among those 13 rays in Eq.(1) determine a graph Δ_{13} with 13 vertices (hollow dots) representing those 13 rays and edges, straight or curved, linking two rays that are orthogonal.

$b|1\rangle + c|2\rangle$. Consider the following 13 rays

$$
\begin{array}{lll}
y_1^- = (0, 1, -1) & h_1 = (-1, 1, 1) & z_1 = (1, 0, 0) \\
y_2^- = (1, 0, -1) & h_2 = (1, -1, 1) & z_2 = (0, 1, 0) \\
y_3^- = (1, -1, 0) & h_3 = (1, 1, -1) & z_3 = (0, 0, 1) \\
y_1^+ = (0, 1, 1) & h_0 = (1, 1, 1) & \\
y_2^+ = (1, 0, 1) & & \\
y_3^+ = (1, 1, 0) & &
\end{array}
\tag{1}
$$

that are determined by 26 points on the surface of a 3×3 magic cube as illustrated in Fig.1. If we regard those 13 rays as 13 vertices and link two vertices if and only if the corresponding rays are orthogonal, then we obtain the orthogonality graph Δ_{13} as shown in Fig.2. Obviously a given set of rays determines uniquely the orthogonality graph and usually not vice versa. However those 13 rays are determined uniquely by the orthogonality relationships specified by the graph Δ_{13} up to a global unitary transformation.

In fact without loss of generality we can choose z_k as in Eq.(1) since they form a basis. Because $\{z_k, y_k^\pm\}$ are mutually orthogonal for each $k = 1, 2, 3$ there exist nonzero t_1, t_2, t_3 such that $y_1^+ = (0, t_1, 1)$ and $y_1^- = (0, -1, t_1^*)$, $y_2^+ = (1, 0, t_2)$ and $y_2^- = (t_2^*, 0, -1)$, $y_3^+ = (t_3, 1, 0)$ and $y_3^- = (-1, t_3^*, 0)$. As a result we have $h_1 = (-t_2^*, t_1, 1)$, $h_2 = (1, -t_3^*, t_2)$, and $h_3 = (t_3, 1, -t_1^*)$. Since h_k is orthogonal to y_{k-1}^+ for $k = 1, 2, 3$ we have $t_1^* = t_2 t_3$, $t_2^* = t_1 t_3$, and $t_3^* = t_1 t_2$ from which it follows that $|t_k| = 1$ and $t_1 t_2 t_3 = 1$, i.e., $t_k = e^{i(\theta_{k+1} - \theta_{k+2})}$ for some real θ_k. Finally we obtain $h_0 = (e^{i\theta_1}, e^{i\theta_2}, e^{i\theta_3})$ which is orthogonal to $y_{1,2,3}^-$. The diagonal unitary transformation taking h_0 to $(1, 1, 1)$ leaves z_k unchanged so that the standard form of 13 rays in Eq.(1) is obtained.

The KS value assignments to the 13-ray set are possible, i.e., no logical contradiction can be extracted by considering conditions 1 and 2 only. However in any possible KS value assignment there is at most one ray among $\{\hat{h}_\alpha | \alpha = 0, 1, 2, 3\}$ that can be assigned to value 1. Sup-

pose that this is not true, i.e., there are two or more $\hat{h}_\alpha$ that are assigned to value 1. Due to the symmetry of the graph Δ_{13} as shown in Fig.2, we need only to consider the following two cases:

i) if $\hat{h}_0$ and $\hat{h}_1$ are assigned to value 1 then $\hat{y}_2^\pm$ and $\hat{y}_3^\pm$ must be assigned to 0 so that both $\hat{z}_2$ and $\hat{z}_3$ must be assigned to value 1 which is impossible;

ii) If $\hat{h}_1$ and $\hat{h}_2$ are assigned to 1 then $\hat{y}_1^\pm$ and $\hat{y}_2^\pm$ must be zero so that both $\hat{z}_1$ and $\hat{z}_2$ must be assigned to value 1, also a contradiction.

In the reasonings above we have taken into account of condition 2 which demands that linked rays not be assigned simultaneously to value 1 and in a triangle one and only one ray be assigned to value 1. A set of eight rays in each case considered above, e.g., $\hat{h}_{0,1}$, $z_{2,3}$, and $y_{2,3}^\pm$, constitutes in fact a 3-box paradox [23] which appears also in Clifton's state-dependent proof of KS theorem [24] and a recent proposal to close the compatibility loopholes [25].

Denoting by $h_\alpha^\lambda \in \{0,1\}$ the value assigned to $\hat{h}_\alpha$ for given λ, we then have $\sum_\alpha h_\alpha^\lambda \le 1$ from the above arguments. As a result the following inequality

$$\sum_{\alpha=0}^3 \langle \hat{h}_\alpha \rangle_c := \sum_{\alpha=0}^3 \int d\lambda \varrho_\lambda h_\alpha^\lambda \le 1 \qquad (2)$$

must be satisfied by all non-contextual HV models that admit a KS value assignment. However the quantum mechanics predicts $\sum_{\alpha=0}^3 \langle \hat{h}_\alpha \rangle_q = 4/3$ due to the identity $\sum_{\alpha=0}^3 \hat{h}_\alpha = \frac{4}{3}I$ with I being the identity operator of qutrit (see Appendix). This proves the original KS theorem: the non-contextual HV model satisfying conditions 1 and 2 cannot reproduce all the predictions of QM on non-sequential measurements.

Usually the KS theorem is proved by finding a set of rays to which the KS value assignment does not exist so that we need not to check other predictions of QM. Our proof here is a set of 13 rays, to which all possible KS value assignments, which do exist, fail to reproduce a certain prediction of QM. Notably the inequality Eq.(2), involving only 4 observables explicitly, provides a state-independent test for the non-contextual HV models that preserve the algebraic structure of compatible observables, in the spirit of Kochen and Specker. In an experimental test of the inequality Eq.(2) each average must be measured on different subensembles prepared in the same state, similar to a standard test of a Bell inequality as pointed out by Cabello [8].

It turns out that the requirement of preserving the algebraic structure, i.e., the product and sum rules, of compatible observables is too strong and unnecessary. Peres already noticed that the sum rule can be abandoned and kept the product rule [27] as in KS proofs via the Mermin-Peres square [19, 26] for 2 qubits and Mermin's pentagram [26] for 3 qubits. However the product rule is not necessary either. Instead we need only

to require that the quantum correlations of compatible observables, the quantum mechanical predictions on sequential measurements, be reproduced. This imposes no additional constraints on the non-contextual HV models since they must reproduce all the predictions of QM in the first place. As noticed earlier, the toy model by Kochen and Specker did not take into account of the quantum correlations of compatible observables.

Indeed every KS proof mentioned previously can be turned into a state-independent KS inequality [9] that is obeyed by all non-contextual HV models, no matter whether the algebraic structure of compatible observables is preserved or not. All known state-independent KS inequality involve the correlations of at least three compatible observables, i.e., predictions on three or more sequential measurements must be reproduced by the HV models. In the case of qutrit the resulting KS inequalities involve too many observables, e.g., at least 31, to be tested experimentally. Recently Klyachko, Can, Binicioglu, and Shumovskya [7] propose a simple KS inequality, called pentagram inequality since it is based on the graph of a pentagon, to test non-contextual HVs with only 5 dichotomic observables and correlations of two compatible observables. However this pentagram inequality, which is based on the assumption of non-contextuality only and whose violation has been verified in a recent experiment [18], has the drawback of being state-dependent.

Our state-independent inequality is based on the orthogonality graph Δ_{13} as shown in Fig.2. We denote by $V = \{y_k^\sigma, h_\alpha, z_k | k = 1,2,3; \sigma = \pm; \alpha = 0,1,2,3\}$ its vertex set and by Γ Its adjacency matrix which is a 13×13 symmetric matrix with vanishing diagonal elements and $\Gamma_{uv} = 1$ if two vertices $u, v \in V$ are neighbors and $\Gamma_{uv} = 0$ otherwise. For arbitrary 13 variables $a_v = \pm 1$ with $v \in V$ it holds

$$\sum_{v \in V} a_v - \frac{1}{4} \sum_{u,v \in V} \Gamma_{uv} a_u a_v \le 8, \qquad (3)$$

which can be easily verified with the help of a laptop by exhausting all 2^{13} possibilities and an analytic proof is provided in Appendix. Let $\{A_v | v \in V\}$ be a set of 13 dichotomic observables taking values $a_v^\lambda = \pm 1$ for given λ. Then from inequality Eq.(3) we obtain our magic-cube inequality

$$\sum_{v \in V} \langle A_v \rangle_c - \frac{1}{4} \sum_{u,v \in V} \Gamma_{uv} \langle A_u \cdot A_v \rangle_c \le 8, \qquad (4)$$

where we have denoted $\langle A_v \rangle_c := \int d\lambda \varrho_\lambda a_v^\lambda$ and $\langle A_u \cdot A_v \rangle_c := \int d\lambda \varrho_\lambda a_u^\lambda a_v^\lambda$. Though the correlation of two observables is always well defined in a non-contextual HV model regardless of whether they are compatible or not, in order to compare with the predictions of QM those observables labeled with linked vertices in the orthogonality graph Δ_{13} should be compatible, i.e, they can be

measured simultaneously or be commuting, so that their correlation is also well defined in QM.

Fortunately if we define 13 observables $\hat{A}_v = I - 2\hat{r}_v$ from 13 rays $\hat{r}_v \in \{\hat{y}_k^\sigma, \hat{h}_\alpha, \hat{z}_k\}$, then $\hat{A}_u$ and $\hat{A}_v$ are commuting. i.e., compatible, whenever two vertices $u, v \in V$ are linked, i.e., $\Gamma_{uv} = 1$. Therefore all the expectation values appear on the left-hand-side of Eq.(4) are also well defined in QM and therefore should be reproduced. Due to the linearity of QM the left-hand-side of Eq.(4) must reproduce the expectation value of

$$\hat{L} = \sum_{v \in V} \hat{A}_v - \frac{1}{4} \sum_{u,v \in V} \Gamma_{uv} \hat{A}_u \hat{A}_v. \qquad (5)$$

Simple calculations yield $\hat{L} = \frac{25}{3} I$ and therefore $\langle \hat{L} \rangle_q = 25/3 > 8$ for any qutrit state, meaning that the magic-cube inequality Eq.(4) is violated by all qutrit states. Thus we have proved in a state-independent fashion that every non-contextual HV model, no matter whether the algebraic structure of compatible observables is preserved or not, cannot reproduce all the predictions of QM, especially those quantum correlations of two compatible observables, by using only 13 observables.

To summarize, our magic-cube inequality Eq.(4) provides the simplest state-independent proof of quantum contextuality: Firstly it is a test for the contextuality for an indivisible system capable of exhibiting the quantum contextuality, i.e., smallest system; Secondly it involves a smallest number of observables so far and we conjecture that KS theorem does not have a state-independent proof with less than 13 rays; Thirdly only correlations of at most two, the smallest number, of compatible observables are involved so that only two observables have to be measured sequentially. In comparison correlations of at least three compatible observables are involved in all the state-independent tests of contextuality known so far. If we impose a minimal requirement on the non-contextual HV models, i.e, only the correlations of at most two compatible observables are required to be reproduced, then our magic-cube inequality will be the first state-independent proof of KS theorem in this case. We believe that there are also proofs of KS theorem for higher dimensional systems that involve only two-observable correlations. Finally we have proved the KS theorem by finding a 13-ray set, which is the smallest state-independent proof so far, for which all possible KS value assignments, which do exist, fail to reproduce a certain prediction of QM. Since only a relatively small number of observables and correlations of only two compatible observables are involved, an experimental test of our inequality is well within the reach of the current technologies. We believe that the nitrogen-vacancy center in diamond [28] should be a promising choice to test our inequality.

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Appendix

Explicit rays for Eq.(1)— By denoting $\bar{1} = -1$ we have

$$\hat{y}_1^\pm = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & \pm 1 \\ 0 & \pm 1 & 1 \end{pmatrix}, \ \hat{y}_2^\pm = \frac{1}{2}\begin{pmatrix} 1 & 0 & \pm 1 \\ 0 & 0 & 0 \\ \pm 1 & 0 & 1 \end{pmatrix}, \ \hat{y}_3^\pm = \frac{1}{2}\begin{pmatrix} 1 & \pm 1 & 0 \\ \pm 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\hat{h}_0 = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \ \hat{h}_1 = \frac{1}{3}\begin{pmatrix} 1 & \bar{1} & \bar{1} \\ \bar{1} & 1 & 1 \\ \bar{1} & 1 & 1 \end{pmatrix}, \ \hat{h}_2 = \frac{1}{3}\begin{pmatrix} 1 & \bar{1} & 1 \\ \bar{1} & 1 & \bar{1} \\ 1 & \bar{1} & 1 \end{pmatrix}, \ \hat{h}_3 = \frac{1}{3}\begin{pmatrix} 1 & 1 & \bar{1} \\ 1 & 1 & \bar{1} \\ \bar{1} & \bar{1} & 1 \end{pmatrix},$$

$$\hat{z}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \ \hat{z}_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \ \hat{z}_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Thus we have identities

$$\hat{y} := \sum_{k=1}^{3}\sum_{\sigma=\pm} \hat{y}_k^\sigma = 2I, \quad \hat{h} := \sum_{\alpha=0}^{3} \hat{h}_\alpha = \frac{4}{3}I, \quad \hat{z} := \sum_{k=1}^{3} \hat{z}_k = I. \tag{6}$$

Let $\hat{A}_v = I - 2\hat{r}_v$ with $\hat{r}_v \in \{\hat{y}_k^\sigma, \hat{h}_\alpha, \hat{z}_k\}$. Since $24 = \sum_{u,v\in V} \Gamma_{uv}/2$ is the number of the edges in Δ_{13}, $\sum_{u\in V} \Gamma_{uv}$ is the degree of the vertex v, and $\hat{r}_v\hat{r}_u = 0$ if $\Gamma_{uv} = 1$, it holds

$$\begin{aligned}
\hat{L} &= \sum_{v\in V} \hat{A}_v - \frac{1}{4}\sum_{u,v\in V} \Gamma_{uv}\hat{A}_u\hat{A}_v \\
&= 13I - 2(\hat{y}+\hat{h}+\hat{z}) - \frac{I}{4}\sum_{uv}\Gamma_{uv} + \sum_{uv}\Gamma_{uv}\hat{r}_v - \sum_{u,v\in V}\Gamma_{uv}\hat{r}_u\hat{r}_v \\
&= 13I - 2(\hat{y}+\hat{h}+\hat{z}) - 12I + 4(\hat{z}+\hat{y}) + 3\hat{h} \\
&= I + 2(\hat{z}+\hat{y}) + \hat{h} = \frac{25}{3}I. \tag{7}
\end{aligned}$$

Proof of Eq.(4)— There are 9 vertices $\{z_k, y_k^\sigma\}$ of degree 4 and 4 vertices $\{h_\mu\}$ of degree 3 in Δ_{13}, where the degree of a vertex denotes the number its neighbors. Let t be the total number of a_v that take value -1, f be the number of a_v that take value -1 with v being of degree 4, and l be the number of pairs of vertices u, v such that $a_u = a_v = -1$ and $\Gamma_{uv} = 1$. We then have $L = 1 + t + f - 2l$. Since the quadratic term in L is unchanged under replacements $a_v \mapsto -a_v$, we need only to consider $t \le 6$. If $t \le 3$, since $l \ge 0$ and $f \le t$, then we have $L \le 7$. If $t = 4$, then from $f - 2l \le 3$ since it is impossible to have $f = 4$ and $l = 0$, i.e., among any 4 vertices of degree 4 there is at least a connected pair, it follows $L \le 8$, which is attained when $f = 3$ and $l = 0$, e.g., z_1, y_2^-, y_3^+ and h_3. In the case of $t = 5$, if $f = 5$ then $l \ge 2$ so that $L \le 7$. If $f \le 4$ then $l \ge 1$ so that $L \le 8$, which is attained by, e.g., z_1, y_2^-, y_3^+, y_1^- and h_3. In the case of $t = 6$, if $f = 6$ then $l \ge 3$ so that $L \le 7$; If $2 \le f \le 5$ then we have again $L \le 8$ because $l \ge 2$; If $f = 1$ then $L \le 7$ since $l \ge 0$.